Phthalic acid, hexyl 2-(methylthio)phenyl ester

Inchi: InChI=1S/C21H24O4S/c1-3-4-5-10-15-24-20(22)16-11-6-7-12-17(16)21(23)25-18-13-8-9
InchiKey: PCSXTVMEYXNNJQ-UHFFFAOYSA-N
Formula: C21H24O4S
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1SC
Mol. weight [g/mol]: 372.48

Physical Properties

Property code	Value	Unit	Source
gf	-103.22	kJ/mol	Joback Method
hf	-474.38	kJ/mol	Joback Method
hfus	47.15	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.365		Crippen Method
mcvol	290.460	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	3335.00		NIST Webbook
rinpol	3335.00		NIST Webbook
tb	964.56	K	Joback Method
tc	1200.50	K	Joback Method
tf	583.03	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.22	J/mol×K	964.56	Joback Method
cpg	902.37	J/mol×K	1003.88	Joback Method
cpg	912.99	J/mol×K	1043.21	Joback Method
cpg	922.12	J/mol×K	1082.53	Joback Method
cpg	929.79	J/mol×K	1121.85	Joback Method
cpg	936.04	J/mol×K	1161.18	Joback Method
cpg	940.88	J/mol×K	1200.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume